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Model prediction on the characteristics of dipole atoms: the concept of Schrodinger's equation

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A B S T R A C T

This paper investigates the model to predict the characteristics of dipole atoms upon the application of Schrödinger's wave equation. Many element of chemists' picture of molecular structure hinge on the point of view that separates the electronic motions from the vibration/rotational motion and treats coupling between these separated motions as perturbations. It is essential to understand the origins and limitations of this separated (dipole) motion picture. To develop a framework in terms of which to understand when such separable is valid, one think of an atom or molecule as consisting of a collection of N electrons and M nuclei each of which possesses kinetic energy and among which columbic potential energies of interaction arise to properly describe the motion of all these particles, one need to consider the full Schrödinger Equation $H\varphi = \in\varphi$ in which the Hamiltonian H contains the sum of the Kinetic energies of all N electron and the M nuclei. The range of accuracy of this separation can be understood by considering the differences in time scales that relate to electronic motions and nuclear motions under ordinary circumstances.

Capsule Summary: This paper investigates the model to predict the characteristics of dipole atoms upon the application of Schrödinger's wave equation.

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INTRODUCTION

A dipole is a separation of opposite electrical charges. This is quantified by its dipole moment (μ). A dipole moment is the distance between charges multiplied by the charge. The unit of the dipole moment is the Debye, where 1 Debye is 3.34 x 10^{-30} cm. The dipole moment is a vector quantity that has both magnitude and direction. The direction of an electric dipole moment points from the negative charge toward the positive charge. Dipole is a molecule that has both positive and negative regions. Although we talk, as though electrons distribute their time evenly among all atoms in a molecule (Stroud, 2007; Ukpaka, 2014).

It is not flexible talking about dipole without a dipole force. Dipole – dipole force is when the positive side of a polar molecule and the negative side come together to form a bound. In order for this kind of bond to work, the molecules need to be very close to each other, like they are in a liquid. A dipole can also be said to be a pair of equal and oppositely charged or magnetized poles separated by a distance (Metha, et al., 2007; Ukpaka, 2017). There are two kinds of dipole: The electric dipole: This is a separation of positive and negative charges of equal magnitude but opposite sign,

separated by some usually small distance. The magnetic dipole: This is a close circulation of electric current. A simple example of this is a single loop of wire with some constant current through it (Riley, et al., 2002).

Dipole can be characterized by their dipole moment which is a vector quantity. For simple electric dipole moment considerable theoretical and experimental interest (Ukpaka and Ndor, 2013). It has been shown that the electron dipole field is capable of supporting an infinite number of bound states for an electron if the dipole moment is greater than the critical values 0.6393 au. Under these circumstances, the excess electron will be bound to the molecular dipole field,

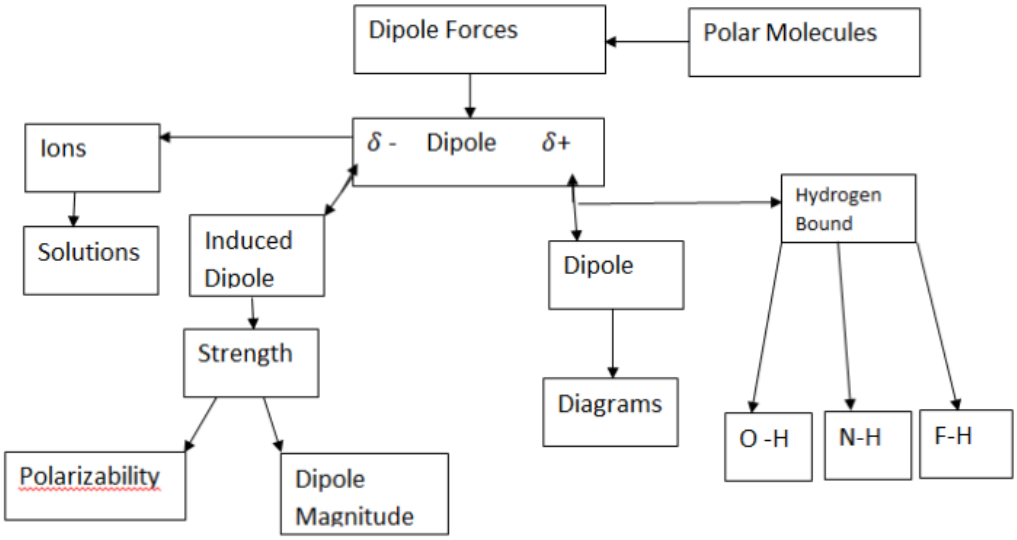

Fig. 1: Systematic algorithm for dipole force interaction (Riley et al., 2002)

points from negative charge towards the positive charge has a magnitude equal to the strength of charges (Ukpaka, et al., 2011). In definition of dipole moment we consider "the dipole limit" where for example the distance of generating charges should converge too while simultaneously the charge strength should diverge to infinity in such a way that the product remains a positive constant. For the current loop, the magnetic dipole moment points through the loop with a magnitude equal to the current in the loop times the area of the loop. In addition to current loop, the election among two fundamental particles has a magnetic dipole moment (Riley, 2002; Ukpaka, 2012; Stroud, 2007).

A permanent magnetic magnet such as a bar magnet owes its magnetism to the intrinsic magnetic dipole moment of the electron. Dipoles are determine by examining electro negativity, while is the ability of an atom to draw electrons to itself. Also, the interaction of a charged particle with an electric dipole is a fundamental problem which received a lot of attention since the early days of nuclear and molecular physics (Amadi and Ukpaka, 2013).

Later, this interest was fueled by the observation that electron capture by a frozen molecule with a permanent electric dipole moment could takes place if the dipole moment exceeds a certain minimum critical value. Another source of interest came from early experimental work on the scattering of low energy electrons by such molecules, which exhibited peculiar features moreover, the electron binding properties of polar molecules have been the topic of giving rise to the so called dipole-bound anion. The critical dipole moment does not depend on the size of the dipole (Riley et al., 2002). However, if the system is treated dynamically to include the rotational degrees of freedom of the nuclei, the infinite number of bound states for the charged electron in the dipole molecular field reduces to a finite number. From the experimental point of view, the formation of a dipole bound anion has been difficult to observe because the much diffused and loosely bound electron are easily stripped away by thermal collisions and/or by the electron fields to which they are exposed. However, recent experimental advances have made it possible to measure the energy of one dipole bound electron very accurately.

MATERIAL AND METHODS

The Schrodinger wave equation

So far, we have made a lot of progress concerning the properties and interpretation of the wave function, but as yet we have had very little to say about how the wave function may be derived in a general situation, that is to say we do not have on hand a wave equation for the wave function. There is no true derivation of this equation, but its form can be motivated by physical and mathematical arguments at a wide variety of levels of sophistication. Here, we will offer a simple derivation based on what we have learned so far about the wave function.

Table 1: Effects of plank's constant in dipole force analysis

m mass of Hydrochloric acid	t(μs) time in microseconds	φ_x = Cost ($\frac{-h^2}{2m}$)t Wave function
36.46094	2×10^{-8}	1
36.46094	4×10^{-8}	1
36.46094	6×10^{-8}	1
36.46094	8×10^{-8}	1
36.46094	10×10^{-8}	1
36.46094	12×10^{-8}	1

Table 2: Effect of dipoles in molecular interaction

M mass of Hydrochloric acid	t(s) time in microseconds	hyp(μm)	adj(μm)	$\varphi_x = \frac{adj}{hyp}$ ($\frac{-h^2}{2m}$)t Wave function
36.46094	2×10^{-8}	2×10^{-8}	1×10^{-8}	-1.525×10^{-78}
36.46094	4×10^{-8}	3×10^{-8}	2×10^{-8}	-4.148×10^{-78}
36.46094	6×10^{-8}	4×10^{-8}	3×10^{-8}	-6.861×10^{-78}
36.46094	8×10^{-8}	5×10^{-8}	4×10^{-8}	-9.76×10^{-78}
36.46094	10×10^{-8}	6×10^{-8}	5×10^{-8}	-1.266×10^{-77}
36.46094	12×10^{-8}	7×10^{-8}	6×10^{-8}	-1.574×10^{-77}

The Schrodinger equation has two 'forms', one in which time explicitly appears, and so describes how the wave function of a particle will evolve in time. In general, the wave function behaves like a wave, and so the equation is often referred to as the time dependent Schrödinger wave equation (TDSE). The other is the equation in which the time dependence has been 'removed' and hence is known as the time independent Schrödinger equation (TISE) and is found to describe, amongst other things, what the allowed energies are of the particle.

These are not two separate, independent equations. The time independent equation can be derived readily from the time dependent equation. In the following we will describe how the first, time dependent equation can be 'derived', and in then how the second follows from the first. In the discussion of the particle in an infinite potential well, it was observed that the wave function of a particle of fixed energy E could most naturally be written as a linear combination of wave functions of the form: wave equation; which is representing a wave travelling in the positive χ direction, and a corresponding wave travelling in the opposite direction, so giving rise to a standing wave, this being necessary in order to satisfy the boundary conditions.

This corresponds intuitively to our classical notion of a particle bouncing back and forth between the walls of the potential well, which suggests that we adopt the wave function above as being the appropriate wave function.

In deriving the equation, we will start from summing the total energy as stated in equation (1a), thus:

£ = KE + PE (1a)

£=1/2mv²+u (1)

We can also write 1/2 mv² from equation (1) as

£ = ρ^2/2m + u (2)

Introducing a wave function

φ=ei(kx–wt) (3)

d_φ/d_x=ikei(kx–wt)=ikφ (4)

Differentiating again we have

(d^2φ)/⟦dx⟧^2=(ik)2φ (5)

Recalling that, K = p/ħh, Where, k = 2π/λ , P = h/d

Therefore, P = h/2π k, as well as P = ħk

From equation (5), we have

$(ik)^2 = -K^2$ and $K^2 = P^2$

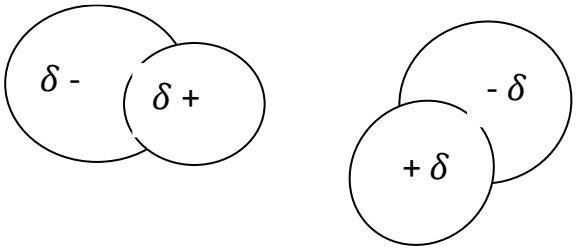

Fig. 2: Showing the dipole force of two hydrochloric acid

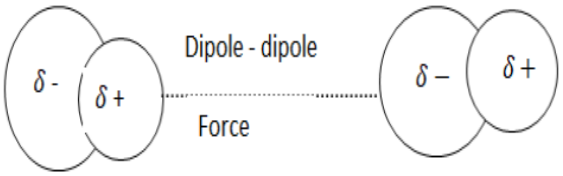

Fig. 3: Reorientation of hydrochloric acid when dipole – dipole force occur (Riley, et al., 2002).

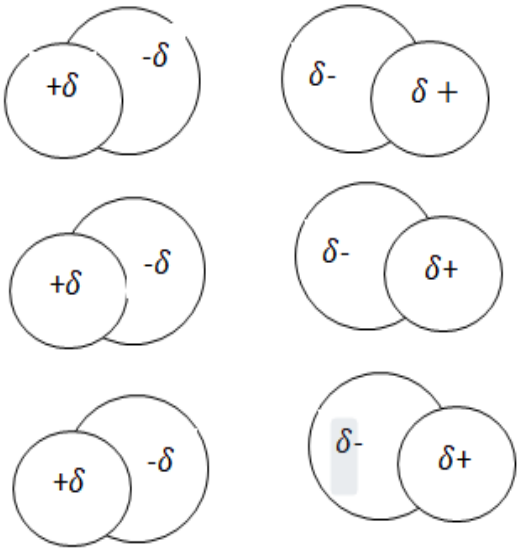

Fig. 4: Hydrochloric molecule before bond molecule (Riley, et al., 2002)

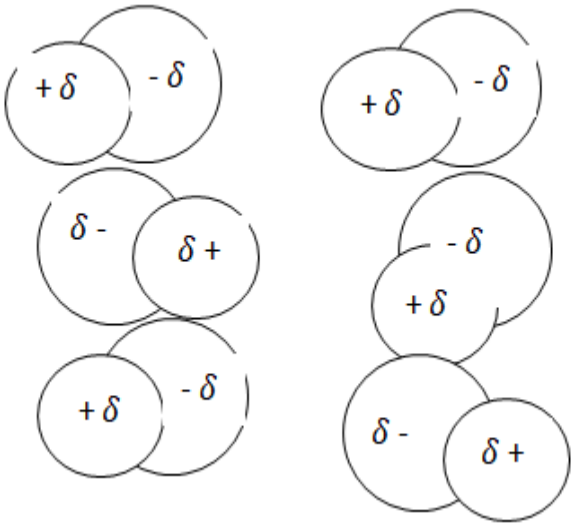

Fig. 5: Normal orientation of hydrochloric (Riley, et al., 2002)

$(d^2\varphi)/[dx]^2=-(P^2/\hbar^2)\varphi$ (6)

Making $P^2\ \varphi$ subject of the formula from equation (6) to the format of equation (2), we have

$-h^2(d^2\varphi)/[dx]^2=P^2\varphi$ (7)

From equation (2), we have

$£=\rho^2/2m+u$ (8)

Multiplying equation (8) through by φ we have

$£\varphi=(\rho^2\varphi)/2m+u\varphi$ (9)

Where, $P^2\ \varphi = -h^2\ (d^2\ \varphi)/[dx]^2$

$t(-h^2)/2m(d^2\ \varphi)/[dx]^2+u\varphi=0$ (10)

Equation (10) is the time independent Schrödinger equation.

Where, £ = Energy, φ = Wave function, h = Planks constants, m = Mass, u = Potential energy

χ = Axis of motion.

We can go further to do the time dependent Schrödinger equation by recalling that

$£ = \hbar w = hf$

If we take φ equation for the wave function, we have

$\varphi = e\ i\ (\ kx - wx)$

And if we differentiate with respect to t, we have

$(d\varphi)/dt=-iw\varphi$ (11)

$£ = \hbar w$

$£\varphi= \hbar w\ \varphi$ (11a)

Dividing through equation (11a) by ħ and multiply the solution equation by –I, we have

$i/\hbar£\varphi=-iw\varphi=d\varphi/dt$ (11b)

$£\ \varphi = \hbar/(-t)\ \ d\varphi/dt$

$£\varphi=i\hbar d\varphi/dt$ (12)

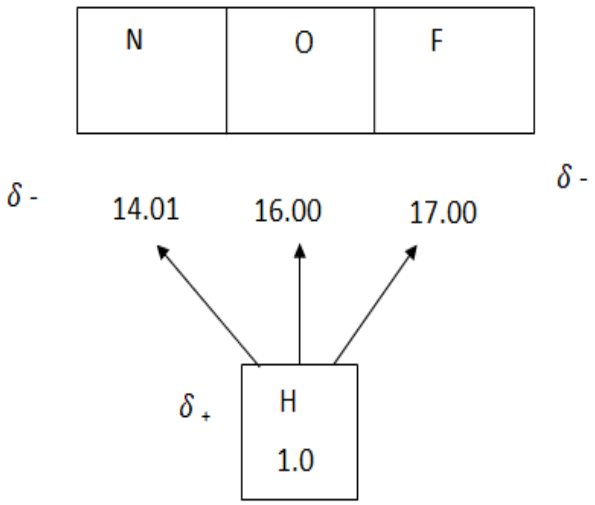

Fig. 6: Example of hydrogen bond with the change Showing hydrogen with positive pole, Nitrogen, oxygen and fluorine with positive pole (Riley et al., 2002).

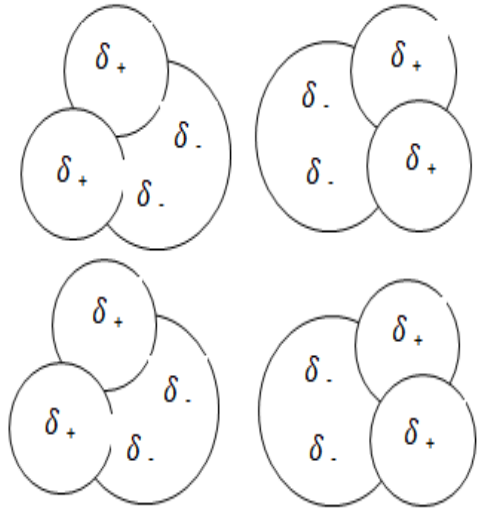

Fig. 7: Water molecule before dipole-dipole type. force reaction (Stroud, 2007)

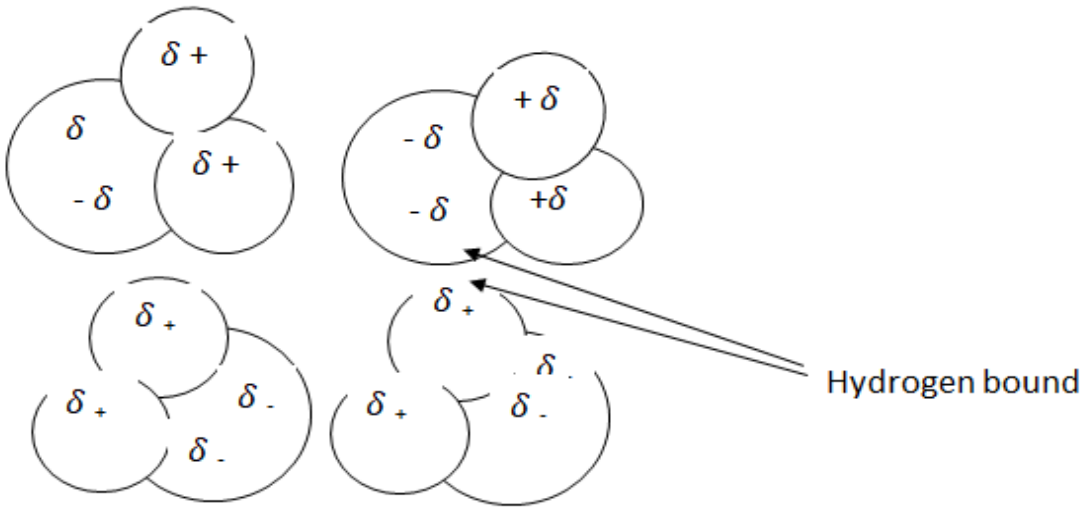

Fig. 8: Showing the orientation of H_2O due to hydrogen bond (Stroud, 2007)

Substituting equation (12) in equation (10), we have

-iħdφ/(d^2t)=(-h^2)/2m(d^2φ)/⟦dx⟧^2+uφ (13)

Equation (13); it's the Time Dependent Schrodinger equation which is the famous time dependent Schrodinger wave equation. It is setting up and solving this equation, then analyzing the physical contents of its solutions that form the basis of that branch of quantum mechanics known as wave mechanics. Even though this equation does not look like the familiar wave equation that describes, for instance, waves on a stretched string, it is nevertheless referred to as a 'wave equation' as it can have solutions that represent waves propagating through space. We have seen an example of this: the harmonic wave function for a free particle of energy £ and momentum P.

Since our focus is basically on the time dependent Schrödinger equation: In general, the solutions to the time dependent Schrodinger equation will describe the dynamical behavior of the particle, in some sense similar to the way that Newton's equation F = ma describes the dynamics of a particle in classical physics. However, there is an important difference. By solving Newton's equation we can determine

the position of a particle as a function of time, whereas by solving Schrodinger's equation, what we get is a wave function "(x, t) which tells us how the probability of finding the particle in some region in space varies as a function of time.

Characteristics of dipole

A polar molecule is characterized by the uneven distribution of the electrons. Forming covalent bonds between each atom in the molecule result in a slightly positively charged side and a slightly negatively charged side. This occurs because of the difference in electro negativity between atoms of different elements. Water (H_2O) is an example of a polar molecule, the oxygen and hydrogen atoms exhibit a force known as dipole-dipole force. Dipole-dipole force is when the positive slid of a polar molecule attracts the negative slide of another polar molecule. In order for this kind of bond to work, the molecules needs to be very close to each other like as they are in liquid. Dipole has many bonds; one of the bonds is hydrogen bond.

Hydrogen bond is an attraction between slightly positive hydrogen on one molecule and a slightly negative atom on another molecule. Hydrogen bonds are dipole-dipole forces, the large electro-negativity difference between hydrogen atoms and several others atoms, such fluorine oxygen and nitrogen, causes the bond between them to be polar, the other atoms have or affinity for the shared electrons, so that they become slightly negatively charged and hydrogen becomes slightly positively charged. Hydrogen atoms are small, so they can cozy up close other atoms. This allows them to come very close to the slightly negatively charged unshared electrons pair of nearby atoms and create a bond with it.

A hydrogen bond is usually represented as a dotted line between the hydrogen and the unshared electron pair of other electronegative atoms. Which are the strongest of all inter molecular forces, they are extremely important affecting the properties of water and biological molecules. Water is a great example of hydrogen bonding. Water is a polar molecule composed of fled hydrogen and one oxygen, the oxygen is slightly negative the hydrogen form hydrogen bonds with the oxygen of adjacent molecules. Then those molecules form more bonds. These bonds maybe respectively weak by themselves but when you have a lot of them together as in the case of water they become very strong.

These bonds help keep water in a liquid state for a wide range of temperatures. Hydrogen bond make water a good solvent because it easily forms hydrogen bonds with others substance.

For Non Polar Molecules, When molecules have an even charge distribution and no dipole moment, then they are non-polar molecules. CO_2 is a linear molecules so our dipole are linear molecules and are symmetrical, the dipole are equal in magnitude but point in opposite direction.

Electro-negativity is the ability of an atom to draw electrons towards it. The potential energy from dipole interaction is important for living organisms. The biggest impact dipole interactions have on living organisms is seen with protein flooding.

RESULTS AND DISCUSSION

In considering forces between two atoms or two molecules in general which are attracted to each other through different aspects including the number of electron that they have is the electron negativity or just depending on the kind of bound they have. But dipole forces depend on the polarity of the molecule i.e. one side of the molecule is going always be slight more negative than the other side of the molecule and the other size of the molecule will be slightly more positive.

Let take Nitroxide (NO) for example, there is always going to be a dipole in the electronegativity when there is two different elements. It negativity is just the tendency of one element to draw the other closer. So in No it happen that oxygen is more electronegativity than nitrogen so it going to be more negative because it attract the electrons

δ + N O δ –

It's just like having a magnet so the negative is obviously going to attract the positive side of another one. As shown below

δ + N O δ - δ + N O δ -

The positive and the negative side are going to join together because of the difference in charges (dipole). In this case we are examining two same molecule which exhibited inter-molecular force and not intra-molecular forces. In terms of the relative strength of the dipole-dipole forces, they are strong but not as hydrogen forces. There are also other components or molecule that experience dipole-dipole force which di-atomic molecule do because there is always going to be a difference in the electron placement within the molecules, e.g Hydrofluoric acid (HF), (ICL), (CO) and (H_2O).

Here the dipole force using the Schrödinger's equation was calculated, which is a time dependent as shown in equation (14) as stated.

$$i\hbar d\varphi/dt=(-\hbar^2)/(2m)(d^2\varphi)/[dx]^2+U\varphi \quad (14)$$

Figure 1 illustrates the systematic algorithm for dipole force interaction (Riley et al., 2002), which was analyzed using the dipole forces concept. Looking at Hydrochloric acid, let sketch out diagrams showing the dipole – dipole forces for easy understanding. Hydrogen is going to have the positive charge and chlorine negative charge. So chlorine will pull the other electron towards itself. What we will get is the dipole – dipole. This will hold hydrochloric acids molecule together before bond was reported by Riley, et al., (2002) and the description of the process is illustrated in (Fig. 4). Although they can never exist like this, so they are joining to orient themselves as. Another specific example is the hydrogen bounds

In the process hydrogen bound is going to occur and we have negative side where oxygen is and positive side where the hydrogen is, so it will orient itself to form.

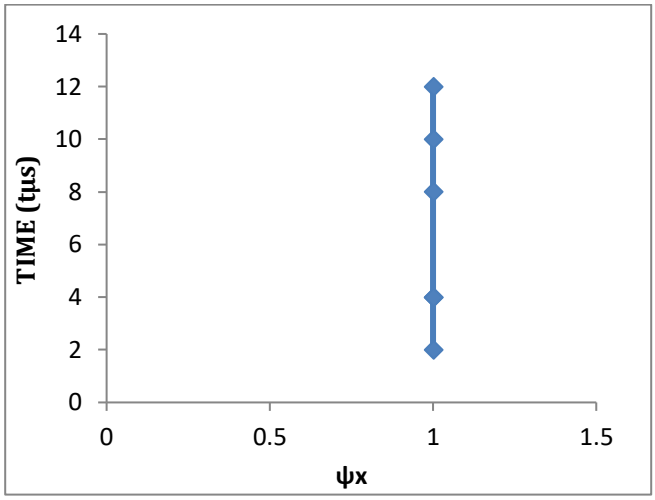

Fig. 9: A graph Time ($t\mu s$) against wave function (φ_x), which shows the influence of plank's constant.

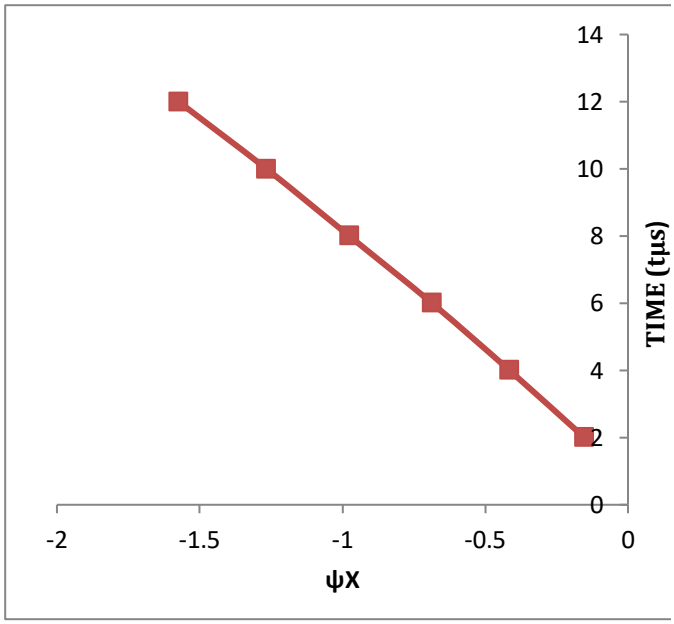

Fig. 10: A graph Time (tμs) against wave function (φ_x), which showing the effects of dipoles in molecular interaction.

Hydrogen bounds are very important because they allow small molecules like water to have pretty good bounds that bond them together. Describing the interaction between molecules; we will be applying the Schrödinger wave equation in the dipole prediction which reads thus.

£φħ^2/2m=-(d^2φ)/⟦dx⟧^2+uφ=0 (15)

Let β = ħ^2/2m

Putting β in equation (15), we have

£φ=β(d^2φ)/⟦dx⟧^2+uφ (16)

β (d^2 φ)/⟦dx⟧^2 + uφ - £φ = 0

β (d^2 φ)/⟦dx⟧^2 + φ (u - £) = 0

Taking the Laplace transformation we have.

(d^2 4)/⟦dx⟧^2=S2φ(s) - S φ(0) – φ^I(0)

φ = φ(s)

β(S2φ(s)–Sφ(0)–φ'(0)+φs(μ-£)=0 (17)

Boundary condition we say let φ'(0) = 0

φ'(0) =1

β[S2φ(s)–S(1)–0]+φs(u-£)=0 (18)

β(S2φ(s)–S+φs(u-£)=0 (19)

βS2φ(s)-βs+φs(μ-£)=0 (20)

From equation (20), let ∝2 = μ - £

βS2φ(s)-βs+φs∝=0 (21)

β S2 φ(s) + φs∝ = βs

φ(s) - (β S2 + ∝) = βs

φ(s)=βs/(βs+∝^2) (22)

From Laplace transform we can say equation (22), we have

φ (t) = Coskt

Where K = β

φt = Cos β t

From equation (15), we have, β (-h^2)/2m

Therefore,

φ_x=Cost((-h^2)/2m)t (23)

Where, t = time (dipole force Orientation process), h = Planks constant, m = mass

From equation (23), let us assume by prediction the time for the reaction (dipole-dipole force) hydrochloric acid at difference instance to be ranging from 2μs, 4μs, 6μs, 8μs, 10μs, 12μs and the mass for hydrochloric is 36.46074g/mol. This graph shows that the plank's constant has great impact in the dipole-dipole force analysis. Secondly from equation (23) lets express cos in terms of cos= adj/hyp and then solving for φ_x, we have

φ_x= (adj/hyp)t((-h^2)/2m)t (24)

CONCLUSIONS

It has been found that a satisfactory wave mechanics can be constructed on the basic of the following auxiliary postulates regarding the nature of wave functions. To be a satisfactory wave function, a solution of the Schrödinger wave equation must be continuous, single-values and finite throughout the configuration space of the system (that is, for all values of the coordinate x which the system can assume). The work has shown how the solution of the Schrödinger equation governing the motion of dipole via dipole-dipole force of an

atom or molecules can be decomposed into two forms such as the time dependent Schrödinger equation and the time independent Schrödinger equation.

This decomposition into approximately separable equation remains an important point of view in this work. It forms the basis of many of our models of molecular structure and our interpretation of molecule. It also establishes how we approach the computational simulation of the dipole force of atoms and molecules. The treatment of dipole motion is cited in section 2, where hydrogen bond case study was used, with the variation of time and distance of the molecules (before attraction), to get a solution for the graph.

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